Scaling Analysis of Random Walks with Persistence Lengths: Application to Self-Avoiding Walks

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Abstract

We develop an approach for performing scaling analysis of N-step Random Walks (RWs). The mean square end-to-end distance, $\langle \vec{R}_N^2 \rangle$, is written in terms of inner persistence lengths (IPLs), which we define by the ensemble averages of dot products between the walker's position and displacement vectors, at the j-th step. For RW models statistically invariant under orthogonal transformations, we analytically introduce a relation between $\langle \vec{R}_N^2 \rangle$ and the persistence length, λ_N , which is defined as the mean end-to-end vector projection in the first step direction. For Self-Avoiding Walks (SAWs) on 2D and 3D lattices we introduce a series expansion for λ_N , and by Monte Carlo simulations we find that λ_∞ is equal to a constant; the scaling corrections for λ_N can be second and higher order corrections to scaling for $\langle \vec{R}_N^2 \rangle$. Building SAWs with typically one hundred steps, we estimate the exponents ν_0 and Δ_1 from the IPL behavior as function of j. The obtained results are in excellent agreement with those in the literature. This shows that only an ensemble of paths with the same length is sufficient for determining the scaling behavior of $\langle \vec{R}_N^2 \rangle$, being that the whole information needed is contained in the inner part of the paths.

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I. INTRODUCTION

Random Walk (RW) models are ubiquitous in the literature with applications in several areas, such as Physics [1], Biology [2] and Economy [3]. The simplest case is the walker displacement in a sequence of independent random steps, namely ordinary RW [4]. One may also obtain random paths on a geometrical space with distinct displacement schemes, leading to other RW models. A fundamental importance of these models lies in the fact that many real phenomena can be mapped or directly represented by paths traversed by walkers in some geometrical space, e.g., a single-strand DNA [5] and magnetic systems [6]. An example is the Self-Avoiding Walk (SAW) defined by a walker forming a random path that never intersects itself; standard SAWs are performed on regular lattices, where the walker steps to nearest-neighbor sites and does not visit a site more than once [7].

Because of non-overlapping paths, the SAW model plays a central role in Polymer Physics [8] by capturing the excluded volume effect in a dilute solution under good solvent condition or at high temperatures [9]. The SAW model is also well known in statistical physics context because of its equivalence with the n-vector model with $n \to 0$, as de Gennes first pointed out [10]. From this equivalence, with arguments of renormalization and field theories, one expects the following series expansion for the mean square end-to-end distance [11, 12]:

$$\langle \vec{R}_N^2 \rangle_N = a_0 N^{2\nu_0} \left(1 + \frac{a_1}{N} + \frac{a_2}{N^2} + \dots + \frac{b_1}{N^{\Delta_1}} + \frac{b_2}{N^{\Delta_1 + 1}} + \dots + \frac{c_1}{N^{\Delta_2}} + \frac{c_2}{N^{\Delta_2 + 1}} + \dots \right), \quad (1)$$

where ν_0 is the leading exponent. The terms proportional to N^{-i} with $i=1,2,\cdots$, are analytical corrections, and the terms proportional to $N^{-(j+\Delta_i)}$ with non-integer exponents $\Delta_i < \Delta_{i+1}$ and $j=0,1,2\cdots$, are the non-analytical corrections to scaling. The leading and corrections to scaling exponents are universal. The indexed brackets $\langle . \rangle_N$ refers to the N-step RW ensemble average, and from now on, unless strictly necessary, we omit the index N. Numerical estimates of exponents ν_0 and Δ_1 are based on either exact counting techniques [13, 14], or in Monte Carlo (MC) simulation methods [15, 16], through the sampling of $\langle \vec{R}_N^2 \rangle$ [17, 18].

Obtaining such estimates for ν_0 and Δ_1 , especially for 3D SAW, is a challenge from several points of view. The exponential growth of the number of possible N-step paths $c_N \approx \mu^N N^{\gamma-1}$, where μ is the connectivity constant and $\gamma > 1$, imposes a limit to exact

counting. To the best of our knowledge, the maximum values obtained are N=79 [19] and N=36 [14] for SAWs on 2D and 3D square lattices, respectively. Concerning Monte Carlo simulations, there exist an appeal to find ν_0 and Δ_1 using very long paths. Obtaining high quality Monte Carlo data for such path lengths is an extremely difficult task for the SAW model. The variable length algorithms suffer from attrition problems, namely barriers that prevent paths to grow, while the fixed length algorithms suffer from the decreasing of acceptance rate to generate a new non-self-intersecting path, according to the increase of the (fixed) path length [20].

Numerical drawbacks also take place when one studies other conformational quantities. An example is the persistence length, λ_N , defined as the mean end-to-end vector projection in a fixed direction along the first step [21, 22], as $N \to \infty$ [23]. Defining the end-to-end vector as $\vec{R}_N = \sum_{j=1}^N \vec{u}_j$, where \vec{u}_j is the walker displacement at the j-th step, the persistence length can be expressed by $\lambda_N = \langle \vec{R}_N \cdot \vec{u}_1 \rangle / |\vec{u}_1| = \sum_{j=1}^N \langle \vec{u}_1 \cdot \vec{u}_j \rangle / |\vec{u}_1|$. Numerical results of λ_N , for 2D-SAWs, are controversial in the literature, and for 3D, are scarce [32]. For 2D-SAW, Grassberger [33] obtained the first estimate of λ_N in the square lattice, by means of a power law $\lambda_N \sim N^{\theta}$, with $\theta = 0.063(10)$. Since for $\theta \approx 0$, it is also well fitted by $\lambda_N \sim \ln(N)$, as suggested by Redner and Privmann [34]. They obtained both estimates by sampling the displacements projections along the first step direction, for all possible configurations of SAW paths with N < 24. This weak divergence has been questioned recently by Eisenberg and Baram [35], because their MC estimates of $\langle \vec{u}_1 \cdot \vec{u}_j \rangle$ show that λ_N converges to a constant when $N \to \infty$. One could employ λ_N in Monte Carlo [28] and experimental characterization of certain polymers [29, 30], despite there exist some limitations of λ_N measures such as divergence and edge effects [31].

Refined results about the scaling behavior of the aforementioned conformational quantities to study universality are challenging, and have been the subject of discussion for many years [11, 15]. As usually one does not have exact results for the SAW model, there exists an appeal for simulations of large, sometimes very large, paths. Here, one proposes to answer two questions about a SAW: (i) What is the asymptotic limit of its persistence length? (ii) Is there some way to find out its scaling behavior employing relatively small chains? To answer these questions, we found an approach for performing scaling analysis of RWs, by focusing in the behavior of $\langle \vec{R}_N^2 \rangle$.

The structure of the paper is as follows: In Sec. II we present the analytical results by

defining the inner persistence length and their relation with $\langle \vec{R}_N^2 \rangle$ and λ_N , for RW models statistically invariant under orthogonal transformations. In Sec. III we provide a series expansion for λ_N and obtain the scaling behavior of 2D and 3D-SAW models with Monte Carlo simulations; we also obtain reliable estimates of the exponents ν_0 and Δ_1 and discuss the contribution of λ_N to $\langle \vec{R}_N^2 \rangle$ behavior. In Sec. IV we give concluding remarks.

II. INNER PERSISTENCE LENGTH AND ANALYTICAL RESULTS

We define the inner persistence length (IPL) for an N-step RW, by the average dot product: $\mathcal{I}_j \equiv \langle \vec{R}_j \cdot \vec{u}_j \rangle$. To relate $\langle \vec{R}_N^2 \rangle$ to \mathcal{I}_j , and \mathcal{I}_N to λ_N , we write the square distance at the j-th step for an N-step RW as: $\vec{R}_j^2 = \vec{R}_{j-1}^2 + 2\vec{R}_j \cdot \vec{u}_j - u_j^2$. Adding up \vec{R}_j^2 , we have $\sum_{j=1}^k \vec{R}_j^2 = \sum_{j=1}^k \vec{R}_{j-1}^2 + \sum_{j=1}^k 2\vec{R}_j \cdot \vec{u}_j - \sum_{j=1}^k |\vec{u}_j|^2$, where $\vec{R}_0 = \vec{0}$ leads to $\sum_{j=1}^k \vec{R}_{j-1}^2 = \sum_{j=1}^{k-1} \vec{R}_j^2$. Thus, considering $|\vec{u}_j| = 1$, we write the average $\langle \vec{R}_k^2 \rangle = 2\sum_{j=1}^k \mathcal{I}_j - k$. In particular for k = N, the mean square end-to-end distance is

$$\langle \vec{R}_N^2 \rangle = 2 \sum_{j=1}^N \mathcal{I}_j - N. \tag{2}$$

Now, consider a generic class of RWs, where ensembles of N-step walks obey the following invariance property: the probability distributions, of each step \vec{u}_i , i=1,2,...,N, which compose a path, is invariant under orthogonal transformations. With this, we exclude walks like the tourist model [36], where the medium disorder [37] breaks down such invariance symmetries. Particularly, one considers an ensemble of N-step RWs obeying the mentioned probabilistic symmetry, under a specific orthogonal transformation T given by $\vec{u}_i \stackrel{T}{\to} \vec{u}'_{N-i+1}$; the prime denotes the displacement vectors in the transformed reference frame, and $\vec{u}'_i = -\vec{u}_{N-i+1}$, with i=1,2,...N. Notice that $\vec{u}'_i \in \{\vec{u}_1,\vec{u}_2...\vec{u}_N\}$, where $\{.\}$ represents the complete ensemble of paths. This symmetry operation can be achieved by a translation followed by inversion of all displacement vectors. In other words, one does invert each path and change the origin to the end of the walk. An immediate consequence for the complete ensemble of random paths is $\{\vec{u}_i\} = \{\vec{u}'_i\}$, with i=1,2,...N, which leads to $\{\vec{R}_N\} = \{\vec{R}'_N\}$. From the previous relations, it follows that $\{\vec{R}_N \cdot \vec{u}_N\} = \{\vec{R}_N \cdot \vec{u}_1\}$, so the configurational average $(\vec{R}_N \cdot \vec{u}_N) = (\vec{R}_N \cdot \vec{u}_1)$ holds. This average, for $N \to \infty$, is the persistence length λ_N . Therefore, the mean square end-to-end distance could be rewritten as

$$\langle \vec{R}_N^2 \rangle = \langle \vec{R}_{N-1}^2 \rangle + 2\lambda_N - 1, \tag{3}$$

and we have established a relation between $\langle \vec{R}_N^2 \rangle$ and λ_N . We observed Eq. 3 numerically, prior to its proof, by exact calculations for $N \leq 24$. Some RW models that obey such a relation are the N-step ensemble of ordinary RW and SAW paths.

III. NUMERICAL RESULTS FOR THE SAW MODEL

From now on, we numerically study \mathcal{I}_j for SAWs using the non-reversed random walk (NRRW) algorithm to generate the ensemble of N-step non-overlapping paths. Because of the attrition problem, i.e., barriers or traps that prevent paths to achieve N steps, the NRRW is inefficient to generate good statistics for long SAWs, since the probability decays as $p_N \propto \exp[-\gamma N]$, where $0 < \gamma < 1$ is the attrition constant. However, the generated data with this algorithm are surprisingly good enough to validate our approach, showing that we choose the right corrections to scaling terms in the expansion of IPLs.

Starting with $\langle \vec{R}_N^2 \rangle$, we now analyze the persistence length. For the square lattice, $\nu_0 = 3/4$ [38] and a common belief is that $\Delta_1 = 3/2$ [40]. With these exponents values, from Eq. 1, using only the first two leading exponents, we see that $\langle \vec{R}_N^2 \rangle \approx AN^{3/2} + BN^{1/2}$. The same reasoning leads to a similar result for cubic lattices, where $\nu_0 \sim 0.587597(7)$ and $\Delta_1 \sim 0.528(12)$ are widely accepted values [17]. Both averages in Eq. 3, $\langle \vec{R}_N^2 \rangle$ and $\langle \vec{R}_{N-1}^2 \rangle$, are obtained considering the same N-step ensemble. In this sense, we follow our previous notation by omitting the bracket index. The difference $\langle \vec{R}_N^2 \rangle - \langle \vec{R}_{N-1}^2 \rangle$ seems to be the discrete derivative of square end-to-end distance, which is not true for the SAW model. One should evaluate the derivative considering SAW ensembles of N and (N-1)-steps: $\langle \vec{R}_N^2 \rangle_N - \langle \vec{R}_{N-1}^2 \rangle_{N-1}$. According to Eq. 1, the leading term of $\langle \vec{R}_N^2 \rangle_N$ derivative is $N^{2\nu_0-1}$ with the first two corrections proportional to $N^{2\nu_0-2}$ and $N^{2\nu_0-\Delta_1-1}$, respectively. From the persistence length plots in Fig. 1, λ_N clearly does not diverge as the leading term of $\langle \vec{R}_N^2 \rangle$ derivative, instead it seems to converge to a constant as N goes to infinity [39]. Thus, we introduce the following series expansion:

$$\lambda_N = \alpha_0 + \alpha_1 N^{-w_1} + \alpha_2 N^{-w_2} + \cdots \tag{4}$$

where the exponents $w_i > 0$, $i = 1, 2, 3 \cdots$, are linear combinations of ν_0 with analytical and non-analytical corrections to scaling exponents. As for example, from the persistence length data fitting with Eq. 4 (see Fig. 1), we find that $w_1 = 2\nu_0 - 2$ and $w_2 = 2\nu_0 - \Delta_1 - 1$

TABLE I. Coefficients and exponents for fitting, with Eq. 4, the λ_N data obtained from simulations for 2D and 3D square lattices. The $w_1 = 0.34(5)$ value is an effective exponent, thus depending on the coefficients α_i and exponents w_i of Eq. 4 [40].

d	$lpha_0$	$lpha_1$	$lpha_2$	w_1	w_2
2	2.525(4)	-2.32(3)	0.81(3)	0.5	1
2^{a}	2.664(3)	-1.714(9)	_	0.34	_
3	1.422(1)	-0.39(6)	-0.022(5)	0.8248	0.34

^a Fitting with equation $\lambda_N \sim \alpha_0 + \alpha_1 N^{-0.34(5)}$ from Ref. [35].

are the best choices. The α_i and w_i values are shown in Tab. I. An immediate consequence of such findings along with Eq. 3, is that λ_N could contribute only with second and higher-order of analytic and non-analytic corrections for $\langle \vec{R}_N^2 \rangle$. Our estimate of λ_N , for square lattices, is compatible with the one of Eisenberg and Baram [35]. Through their estimate of the step-step correlation scaling: $\langle \vec{u}_1 \cdot \vec{u}_j \rangle = \langle \xi_{1,j} \rangle_N \sim 0.6 j^{-1.34(5)}$, and the definition $\lambda_N = \sum_{j=1}^N \langle \xi_{1,j} \rangle_N$, we obtained $\lambda_N \sim \alpha_0 - 1.7 N^{-0.34(5)}$, with which we fitted the persistence length data, but leaving α_1 free, as shown in the inset of Fig. 1(a).

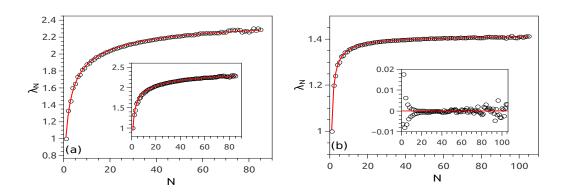


FIG. 1. SAW persistence length for (a) square and (b) cubic lattices. In both lattices, λ_N converges to a constant. The inset plot (a) shows λ_N fitted by the function $\alpha_0 + \alpha_1 N^{-0.34}$ of Ref. [35], where $\lambda_{\infty} = 2.664(3)$ is compatible with our estimate $\lambda_{\infty} = 2.525(4)$ from Eq. 4. For the cubic lattice, $\lambda_{\infty} \sim \sqrt{2}$ is compatible with the one of Ref. [32]. The inset plot (b) depicts the random pattern of the residual plot for λ_N when fitted by Eq. 4.

Now, consider \mathcal{I}_j , for 1 < j < N. According to the collapsed $\log \times \log$ plots of Fig. 2, it is

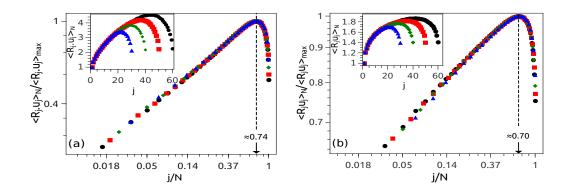


FIG. 2. IPL data collapse in log-log scale for (a) square and (b) cubic lattices with ($\blacktriangle N = 30$), ($\blacklozenge N = 40$), ($\blacksquare N = 50$) and ($\blacklozenge N = 60$). The $\langle \vec{R}_j \cdot \vec{u}_j \rangle_N$ behaves as linear increasing function up to $\sim j_{max}$, with a slope $\approx (2\nu_0 - 1)$. In both lattices $j_{max} \propto N$, with constant of proportionality close to each other (~ 0.7). For $j > j_{max}$ the scalar products contribute to residual terms of corrections to scaling of $\langle \vec{R}_N^2 \rangle$.

notable that \mathcal{I}_j looks like a straight line up to near the point where it reaches its maximum value, at the j_{max} step, with a positive slope $\approx 2\nu_0 - 1$. From Eqs. 1 and 2, and Fig. 2, assuming \mathcal{I}_j scales as $j^{2\nu_0-1}$ is reasonable, at least for $j < j_{max}$. Such proportionality leads us to look for reliable estimates of ν_0 , and corrections to scaling exponents, for SAW ensembles with N not too large. To accomplish this aim, diminishing the influence of the N-step ensemble on estimates of scaling exponents is necessary. In other words, it is necessary to find a cutoff step $j = j_c(N)$, at which \mathcal{I}_j begins to be noticeably influenced by the N-step SAW ensemble. Surely, we can neglect steps above j_{max} . To seek the $j_c(N)$ step, we use the difference between the IPLs of two N-step ensembles, one that contains N_1 , and the other N_2 steps,

$$\Delta R_j(N_1, N_2) = \langle \vec{R}_j \cdot \vec{u}_j \rangle_{N_2} - \langle \vec{R}_j \cdot \vec{u}_j \rangle_{N_1}, \tag{5}$$

where $N_2 > N_1$. According to Fig. 3(a), the IPL has approximately the same behavior for the two path lengths, up to the middle of the shortest path, $j_c(N_1) \sim N_1/2$, for square lattices. Similarly, for cubic lattices, it has the same behavior, up to a third of the shortest path $j_c(N_1) \sim N_1/3$ [see Fig. 3(b)]. Therefore, using $j \leq j_c(N)$, with $j_c(N) = N/2$ and $j_c(N) = N/3$ for 2D and 3D lattices, respectively, it is suitable to estimate the scaling exponents through \mathcal{I}_j .

Additional information to do scaling analysis with \mathcal{I}_j comes from the expansion of $\langle \vec{R}_N^2 \rangle$

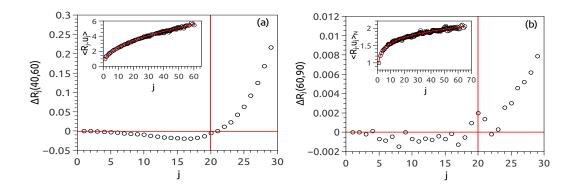


FIG. 3. IPL differences $(\Delta R_j(N_1, N_2))$ for SAWs: (a) for square and (b) cubic lattices, with $N_1 = 40$ and $N_2 = 60$, and $N_1 = 60$ and $N_2 = 90$, respectively. According to $\Delta R_j(N_1, N_2)$ depicted here [see Eq.5], the \mathcal{I}_j starts to be influenced for $j_c > N_1/2$ and $j_c > N_1/3$, for 2D and 3D square lattices, respectively. Inset plots show IPL non-weighted fit using Eq. 6, within a confidence interval of 95%. The square lattice data includes N ranging from 90 to 120 with increment of 10. The fitting parameters obtained are $\varphi = 0.4979(21)$ and $\beta_1 = 0.6630(50)$. The cubic lattice data includes N ranging from 150 to 195 with increment of 15. The fitting parameters obtained are $\varphi = 0.1752(14)$, $\Delta_1 = 0.522(52)$, and $\beta_1 = 0.7581(56)$.

in powers of N. We have found no evidence of the linear term in the expansion of $\langle \vec{R}_N^2 \rangle$ on square or cubic lattices. The nonexistence of the linear term is also reported in Refs. [41, 42]. From Eq. 2, the only way to disappear with the linear term in the expansion of $\langle \vec{R}_N^2 \rangle$ is if the summation of \mathcal{I}_j cancels it out. This finding, with Eq. 1, leads us to write

$$\mathcal{I}_{j} = \beta_{0} + \beta_{1}(j - \tau)^{\varphi} \left[1 + \beta_{2}(j - \tau)^{-\Delta_{1}} + \dots \right], \tag{6}$$

for $j \leq j_c(N)$, where τ is a smoothing constant [43]. We set $\beta_0 = 1/2$ just to cancel the linear term. Also, we did another ansatz: $\beta_2 = -(2\nu_0 - 1)$ and $\tau = 0.5$. This was inspired by results considering only the first non-analytical correction to scaling term, and leaving only the parameters β_1 , β_2 and τ free, which lead us to find $\beta_2 \approx -(2\nu_0 - 1)$ for the 3D case. Notice that, in general $\beta_1 = \beta_1(N)$ and $\beta_2 = \beta_2(N)$; however, for N not too large, order of hundreds for 2D and 3D cases, these parameters converged to constants, for $j \leq j_c(N)$.

The IPL data, containing several N-step ensembles, fitted by Eq. 6 is depicted in the inset plots of Fig. 3. For both, the 2D and 3D square lattices, the leading and sub-leading exponents are in excellent agreement with the believed results. For the square lattice, we found $\nu_0 = 0.7489(21)$, and the non-analytical first exponent results in $\Delta_1 = 3/2$; because it

does not appear in Eq. 6, showing that there exists a constant in the expansion of $\langle \vec{R}_N^2 \rangle$. This is confirmed through the expansion of λ_N ; the predicted results are $\varphi=0.5$ and $\Delta_1=3/2$. For cubic lattices we found $\nu_0=0.58757(140)$, and $\Delta_1=0.522(52)$, while the best predicted results are $\nu_0=0.587597(7)$ and $\Delta_1=0.528(12)$ [17]. Using several N-step ensembles seeks to reduce the error on exponent estimates; however, they may carry some small biased errors. To check this, for 2D-SAW, we used N=120 steps obtaining $\nu_0=0.7500(63)$, and for 3D-SAW we used N=198 steps giving $\nu_0=0.58758(450)$ and $\Delta_1=0.52(17)$. However, the errors we get are not as small as those from literature for the 3D case [17]. We can improve these results, by taking into account the advantage of the statistical invariance, and calculating the IPL starting from the end of the generated chains, thus doubling the sample. In fact, it is out of the scope of this paper to find high precision values for the exponents, but to validate and evaluate the benefits of our approach. Moreover, the whole potential of the method to do the scaling analysis of RWs has not been fully exploited. We expect that the corrections to scaling exponents are easily accessible from the study of the monotonically decreasing \mathcal{I}_j terms of $\langle \vec{R}_N^2 \rangle$, which will readily be tackled.

IV. CONCLUDING REMARKS

In summary, we have proposed an approach to address the scaling of RW conformational quantities, where the mean square end-to-end distance is proportional to the summation of the inner persistence length, $\mathcal{I}_j = \langle \vec{R}_j \cdot \vec{u}_j \rangle$. For RW models, where paths obtained by orthogonal transformations occur with the same probability, we obtained a novel relation between the mean square end-to-end distance and persistence length. Despite the numerical limitations to do scaling analysis, we introduce a series for the persistence length λ_N and show that it converges to a constant, α_0 , apart corrections to scaling terms. We also developed a method to calculate the scaling exponents from \mathcal{I}_j with a path cutoff that diminishes the N-step ensemble influence. Thus, the method is efficient to obtain the scaling behavior of SAW.

We conclude that only an ensemble of paths with the same length is sufficient for performing scaling analysis, being that the whole information needed are contained in the inner part of the paths. The scaling method discussed in this paper can be important for studying universality, criticality, and conformational properties of systems mapped on RW models, such as polymers, biopolymers, and magnetic systems.

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